Dimefox
115-26-4 | DTXSID8041870

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 58.1 °C

Global applicability domain: Inside

Local applicability domain index: 3.65e-01

Confidence level: 3.99e-01

Nearest Neighbors from the Training Set

Image not found
Boranediamine, 1-fluoro-
N,N,N',N'-tetramethyl-
Measured: -44.3
Predicted: -16.9

Image not found
1,3-Dichloro-5,5-
dimethylhydantoin
Measured: 132
Predicted: 133

Image not found
3-Bromo-1-chloro-5,5-
dimethylhydantoin
Measured: 164
Predicted: 158

Image not found
Pyridostigmine bromide
Measured: 153
Predicted: 88.2

Image not found
n-Propyl nitrate
Measured: -100
Predicted: -98.6